$$-N^{-13}C^{\alpha} - ^{13}C' - N - C^{\alpha} - C' - N^{-13}C^{\alpha} \underbrace{ ^{13}C' - ^{15}N }_{-}C^{\alpha} - C' - N - C^{\alpha} - C' - Arg45 - Val49$$

Fig. 1

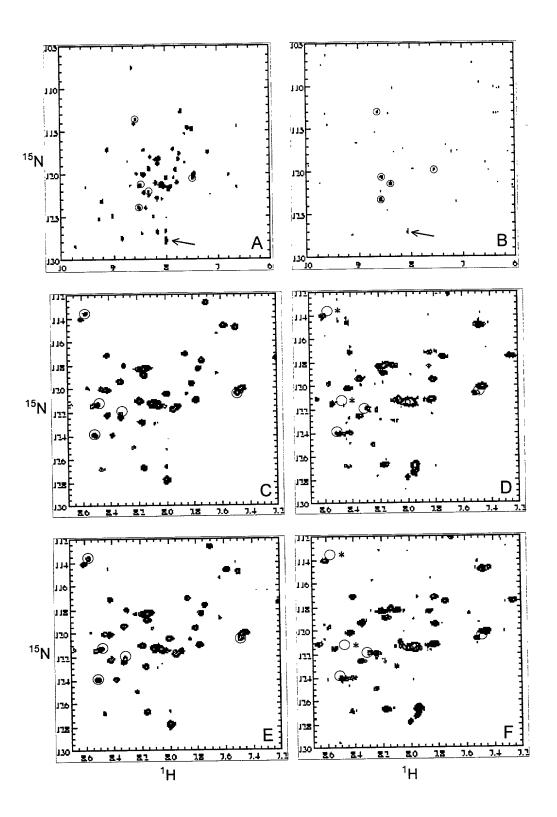


Fig. 2



Fig. 3

Compound	Structure	%	NMR binder
control (no		inhibition 0	-
compound added) N35	HA	14	no
N136	MN N	28	no
N200	444	20	yes
N212	OH CH	0	no
PNU179983	HO.COOH HOSE WHO	100 -X-N H	yes
	HO.C.O.O.S.C.NHO		

Fig. 4

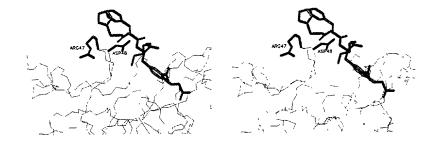
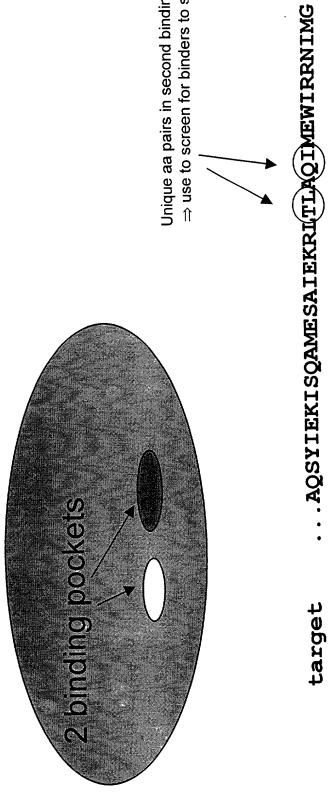


Fig. 5

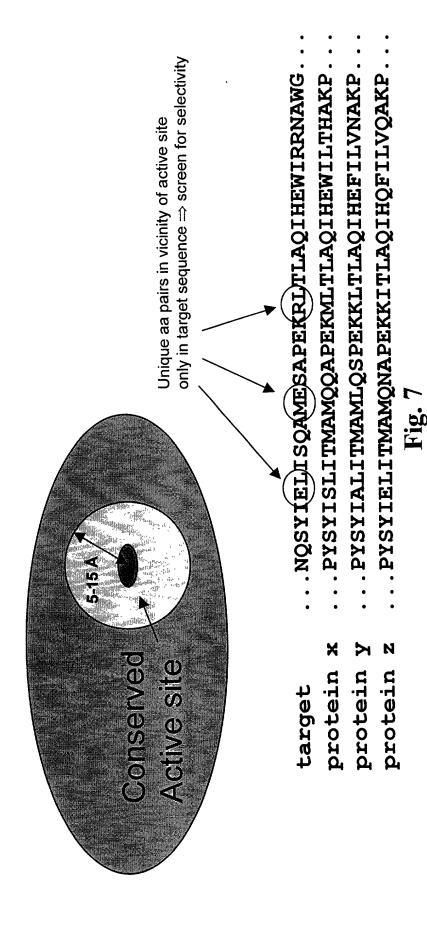
Application I: screen for binding to single binding site



⇒ use to screen for binders to second pocket Unique aa pairs in second binding pocket

Fig. 6

Application II: screen for specificity in vicinity of active site



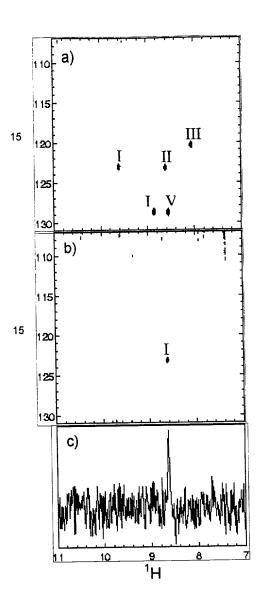


Fig. 8

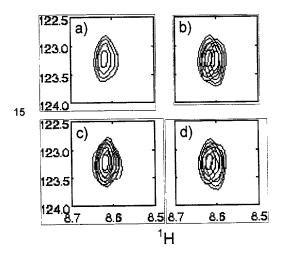


Fig. 9